butyl 1-naphthoate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.36e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.82e-01

Confidence level: 4.22e-01

Nearest Neighbors from the Training Set

Image not found
Oxabentrinil
Measured: 8.61e-05
Predicted: 1.53e-03

Image not found
alpha-Santonin
Measured: 8.12e-04
Predicted: 5.45e-04

Image not found
Siduron
Measured: 7.75e-05
Predicted: 2.20e-03

Image not found
Benquinox
Measured: 2.07e-05
Predicted: 3.02e-02